UDC 551.509.313:551.510.53:551.513:551.557

Design Criteria for Finite-Difference Models for Eddy Diffusion With Winds That Guarantee Stability, Mass Conservation, and Nonnegative Masses

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ABSTRACT—A technique for following the circulation of a tracer in a turbulent fluid is developed from the integral form of the mass continuity equation. Numerical methods based on this technique are shown to be stable, to ensure that the total tracer mass is conserved, and that the mass in any region is always nonnegative. As an illustration of the utility of the technique, a numerical method is developed for a two-dimensional model of the stratosphere.

1. INTRODUCTION

Consider a substance ("tracer") initially fed into a localized region of a fluid in turbulent motion. The time rate of change of the spatial distribution of the tracer is determined by the mass current, $\mathbf{j}$, of the tracer, where

$$\mathbf{j}=\rho\chi\mathbf{v}. \tag{1}$$

Here, ρ is the density of the fluid, χ is the mass of tracer per unit mass of fluid, and $\mathbf{v}$ is the fluid velocity. If all these quantities are written as the sum of a time average value (over a time that is long compared with the characteristic time of the turbulence) and a fluctuation from this value, eq (1) becomes

$$\bar{\mathbf{j}}+\mathbf{j}'=(\bar{\rho}+\rho')(\bar{\chi}+\chi')(\bar{\mathbf{v}}+\mathbf{v}'). \tag{2}$$

Neglecting fluctuations, ρ', in the fluid density gives

$$\bar{\mathbf{j}}=\rho\bar{\chi}\bar{\mathbf{v}}+\rho\overline{\chi'\mathbf{v}'}. \tag{3}$$

According to the eddy diffusion prescription (Hinze 1959), the last term in this equation may be replaced approximately by a linear function of the components of the gradient of the mean mass ratio $\bar{\chi}$; that is,

$$\bar{\mathbf{j}}=\rho\bar{\chi}\bar{\mathbf{v}}-\rho\mathbf{K}\nabla\bar{\chi}. \tag{4}$$

The first term on the right side of eq (4) represents movement of the tracer by mean motions of the fluid (winds if the fluid is the atmosphere), and the second represents spreading of the tracer by eddy diffusion. In contrast to the molecular diffusion coefficient, which is a scalar, the eddy diffusion coefficients form a second-rank tensor $\mathbf{K}$.

The time evolution of the tracer concentration may be studied using the tracer mass continuity equation. The differential form of the equation is

$$\rho\frac{\partial\bar{\chi}}{\partial t}=-\nabla\cdot\bar{\mathbf{j}}+s \tag{5}$$

where s is the net rate of change of tracer density due to sources and sinks. In any complex system, the time evolution of the tracer mass is generally determined numerically. Most commonly, the numerical method is based upon eq (5). This entails selecting a set of gridpoints throughout the fluid and representing the time and space derivatives at each gridpoint in finite-difference form.

In this paper, however, we consider numerical solutions based on the integral form of the continuity equation, so that only first-order spatial derivatives occur in the expressions obtained for the time dependence of the tracer mass distribution. The region occupied by the fluid is divided into N "boxes". The time rate of change of tracer mass within any box is then equal to the flux through its boundaries plus the net rate of change due to sources and sinks. The fluxes may be calculated from the mass current, $\bar{\mathbf{j}}$. In finite-difference form, the fluxes for a given box may be expressed as linear combinations of tracer masses in the box itself and in adjacent boxes. The coefficients of the tracer masses are then functions only of eddy diffusion coefficients and winds. If each tracer mass within a box is treated as a component of an N-dimensional vector, $\mathbf{m}$, the continuity equation takes the form

$$\frac{d\mathbf{m}}{dt}=\mathbf{A}\mathbf{m}+\mathbf{S}. \tag{6}$$

$\mathbf{A}$ is an $N\times N$ matrix of coefficients α_{ij} depending on eddy diffusion coefficients and winds; the presence of winds makes $\mathbf{A}$ nonsymmetric. $\mathbf{S}$ is an N-vector representing the rate of change of the masses due to sources and sinks.

The time derivative may also be expressed in finite-difference form. Most simple is the first forward-difference approximation

$$\frac{d\mathbf{m}}{dt} \approx \frac{\mathbf{m}(t+\Delta t)-\mathbf{m}(t)}{\Delta t}, \qquad \Delta t>0. \tag{7}$$

Combining this with eq (6) leads to

$$\mathbf{m}(t+\Delta t)=(\mathbf{I}+\mathbf{A}\Delta t)\mathbf{m}(t)+\mathbf{S}(t)\Delta t, \tag{8}$$

where $\mathbf{I}$ is the $N\times N$ unit matrix.

The physical system is such that tracer masses in any region are nonnegative. If the fluid is enclosed by impenetrable boundaries and there are no sources or sinks, then the total tracer mass is conserved. It is difficult to ensure that finite-difference equations based on the differential form of the continuity equation [eq (5)] also exhibit these properties without using some ad hoc correction procedure. As will be demonstrated in section 2, the masses satisfying eq (6) are conserved and nonnegative, provided the coefficients α_{ij} satisfy the following constraints:

$$\alpha_{jj}<0, \qquad j=1, \ldots, N, \tag{9}$$

$$\alpha_{ij}\geq 0, \qquad i,j=1, \ldots, N;\ i\neq j, \tag{10}$$

and

$$\sum_{i=1}^{N} \alpha_{ij}=0, \qquad j=1, \ldots, N. \tag{11}$$

It will also be shown that these constraints ensure the stability of eq (6). By adding a further constraint on Δt [eq (28)], one may show that the properties of conservation and nonnegativity of masses and stability also hold for eq (8).

Our approach is similar in spirit to that of Arakawa (1966) who obtained stability in the numerical solution of the Navier-Stokes equation by requiring the finite-difference scheme to conserve mean kinetic energy and mean square vorticity.

Although numerical models satisfying the appropriate constraints just mentioned are stable and guarantee mass conservation and nonnegative masses, they do not, therefore, necessarily give accurate results. In particular, we do not treat the problem of "spurious diffusion" that arises from the interaction of wind terms with a finite mesh size and leads to dispersion of mass in addition to that due to the diffusion coefficients $\mathbf{K}$. This problem is also present in numerical schemes based on the differential form [eq (5)]. In practice, it can be overcome by using sufficiently small steps in space and time; this is clearly undesirable from an economic viewpoint.

In section 3, we generalize the above to the case with sources and sinks and penetrable boundaries that allow an efflux of tracer. It is found that the third constraint [eq (11)] must be replaced by

$$\sum_{i=1}^{N}\alpha_{ij}\leq 0, \qquad j=1, \ldots, N. \tag{12}$$

In section 4, we consider a two-dimensional system and give an example of a numerical scheme satisfying these constraints. Finally, in section 5, we demonstrate the use of the numerical methods on a two-dimensional model of the stratosphere. The nonnegative property of the masses and conservation of mass are verified, and the mass distribution is shown to converge to the equilibrium state.

2. PROPERTIES OF THE NUMERICAL PROCESSES—NO SOURCES OR SINKS, IMPENETRABLE BOUNDARIES

In this section, we consider eq (6) and (8) with $\mathbf{S}\equiv\mathbf{O}$ and impenetrable boundaries. Constraints (9), (10), and (11) are imposed. We first discuss the conditions of nonnegative tracerm asses and the conservation of tracer mass, and conclude with a discussion of stability.

Nonnegative Tracer Masses

If any inital set of nonnegative tracer masses is allowed in eq (6), constraint (10) is a necessary condition for the masses to remain nonnegative. This can be seen by taking an initial distribution with all tracer mass in the kth box; that is,

$$m_j(t)=m\delta_{jk}, \qquad j=1, \ldots, N. \tag{13}$$

Then, from eq (6),

$$\frac{dm_i}{dt}=\sum_j \alpha_{ij}m_j=m\alpha_{ik}. \tag{14}$$

Constraint (10) is required to ensure that the masses in boxes other than the kth do not decrease.

Similar considerations apply to eq (8). There is, however, an additional constraint on the time step, Δt. If the distribution given in eq (13) is substituted into eq (8), we find

$$m_k(t+\Delta t)=(1+\Delta t\alpha_{kk})m.$$

Since $\alpha_{kk}<0$, a negative mass can be obtained unless

$$\Delta t\leq\frac{1}{|\alpha_{\max}|} \tag{15}$$

where α_{max} is the diagonal element α_{kk} of largest modulus.

Constraints (10) and (15) together form a sufficient condition for nonnegative masses in eq (8). Suppose that at time t all masses are nonnegative. The tracer mass in the ith box at time $t+\Delta t$ is

$$m_i(t+\Delta t)=(1+\Delta t\alpha_{ii})m_i(t)+\Delta t\sum_{j\neq i}\alpha_{ij}m_j(t)$$
$$\geq(1+\Delta t\alpha_{ii})m_i(t)$$

because of inequality (10). Thus, $m_i\ (t+\Delta t)\geq 0$ provided inequality (15) is satisfied. Since eq (6) can be obtained from eq (8) by taking the limit $\Delta t\rightarrow 0$, in which case constraint (15) is automatically satisfied, constraint (10) by itself is a sufficient condition for nonnegative masses in eq (6).

Conservation of Tracer Mass

Suppose that initially all tracer is in the kth box as in eq (13). Except in the trivial case where there is no tranport of tracer, conservation of tracer mass requires the mass in the kth box to decrease. From eq (14) [based on eq (6)], we see that α_{kk} must, therefore, be negative; that is, constraint (9) must hold. Moreover, by summing both sides of eq (14) over i and invoking conservation of tracer mass, we obtain constraint (11); that is,

$$\sum_{i=1}^{N}\alpha_{ik}=0.$$

Both these constraints may also be derived in the same manner from eq (8).

Equation (11) ensures conservation of mass in eq (6) and (8) for any initial distribution of tracer since

$$\sum_i\sum_j\alpha_{ij}m_j=\sum_j m_j\sum_i\alpha_{ij}=0.$$

Therefore, using eq (6), we get

$$\frac{d}{dt}\left(\sum_i m_i\right)=\sum_i\frac{dm_i}{dt}=0,$$

and, using eq (8), we get

$$\sum_i m_i(t+\Delta t)=\sum_i\sum_j(\delta_{ij}+\Delta t\alpha_{ij})m_j(t)$$

$$=\sum_i m_i(t).$$

Stability

Equations (6) and (8), with $\mathbf{S}\equiv\mathbf{O}$, are stable if the tracer mass distribution $\mathbf{m}$ evolves to an equilibrium distribution $\hat{\mathbf{m}}$ given by

$$\mathbf{A}\hat{\mathbf{m}}=0 \tag{16}$$

where the sum of the components of $\hat{\mathbf{m}}$ is equal to the sum of the components of the initial distribution.

Consider first the stability of eq (6). Constraints (9)–(11) together imply that

$$|\alpha_{kk}|=\sum_{j\neq k}|\alpha_{jk}|. \tag{17}$$

It follows from constraint (9) and eq (17) that any eigenvalue λ of the matrix $\mathbf{A}$ satisfies

$$|\lambda-\alpha_{\max}|\leq|\alpha_{\max}| \tag{18}$$

(Varga 1962) where $\alpha_{\max}$ is the diagonal element of $\mathbf{A}$ with the largest modulus; that is, any eigenvalue of $\mathbf{A}$ lies in or on the circle in the complex plane whose center is at $\alpha_{\max}=-|\alpha_{\max}|$ and whose radius is $|\alpha_{\max}|$. In particular, this implies that

$$\mathrm{Re}\ \lambda\leq 0, \tag{19}$$

the equality holding only when $\lambda=0$.

There is at least one zero eigenvalue of $\mathbf{A}$. This follows directly from eq (11), which implies that the transpose, $\mathbf{A}^T$, of $\mathbf{A}$ has an eigenvector with all components equal, corresponding to a zero eigenvalue.

Let a new set of mass variables $\mathbf{m}'$ be defined by a nonsingular linear transformation

$$\mathbf{T}\mathbf{m}'=\mathbf{m}. \tag{20}$$

In the transformed equations of motion, the matrix of coefficients is

$$\mathbf{A}'=\mathbf{T}^{-1}\mathbf{A}\mathbf{T}. \tag{21}$$

$\mathbf{T}$ may be chosen so that $\mathbf{A}'$ is in Jordan canonical form, consisting of nonzero blocks (submatrices) along the diagonal and zero blocks elsewhere. The lth block has all its diagonal elements equal to one particular eigenvalue λ_l of $\mathbf{A}$ (or $\mathbf{A}'$), all elements directly above the diagonal equal to unity, and all other elements equal to zero. The transformed equations of motion consist of a number of independent sets of differential equations, one for each block. The part of $\mathbf{m}'$ lying in a block with eigenvalue Re $\lambda<0$ tends to zero as $t\rightarrow\infty$ (Bellman 1960).

If ξ denotes the part of $\mathbf{m}'$ corresponding to a block with $\lambda=0$, then

$$\dot{\xi}=\mathbf{C}\xi \tag{22}$$

where $\mathbf{C}$ is a matrix with all elements directly above the diagonal equal to unity and all other elements equal to zero. If $\mathbf{C}$ is $r\times r$, then $\mathbf{C}^r=0$ and $\mathbf{C}^{r-1}$ has all elements equal to zero except for a one in its top right corner.

The solution of eq (22) with initial value $\xi(0)$ is

$$\xi(t)=e^{\mathbf{C}t}\xi(0)=\sum_{n=0}^{\infty}\frac{(\mathbf{C}t)^n}{n!}\xi(0)=\sum_{n=0}^{r-1}\frac{\mathbf{C}^nt^n}{n!}\xi(0). \tag{23}$$

For large t, the dominant term [except for special $\xi(0)$] is the term in t^{r-1}; that is,

$$\frac{\mathbf{C}^{r-1}}{(r-1)!}t^{r-1}\xi(0). \tag{24}$$

If $r>1$, the magnitude of expression (24) tends to infinity as $t\rightarrow\infty$. The magnitude of the corresponding vector of masses $\mathbf{m}(t)$ also tends to infinity. This contradicts conservation of total mass, hence $r=1$. That is, each zero eigenvalue of $\mathbf{A}$ is associated with a 1×1 Jordan block, and eq (22) becomes

$$\dot{\xi}=0. \tag{25}$$

The equation of motion [eq (6)] is therefore stable.

The stability of eq (8) may be analyzed with the help of the same transformation to oblique coordinates $\mathbf{m}'$. The transformed equation of motion is

$$\mathbf{m}'(t+\Delta t)=(\mathbf{I}+\mathbf{A}'\Delta t)\mathbf{m}'(t). \tag{26}$$

If ξ is the part of $\mathbf{m}'$ corresponding to a zero eigenvalue of $\mathbf{A}'$, then it corresponds to an eigenvalue 1 of $\mathbf{I}+\mathbf{A}'\Delta t$. Accordingly, ξ is constant; that is,

$$\xi(t+\Delta t)=\xi(t).$$

Let us now consider the other parts of $\mathbf{m}'$ corresponding to Jordan blocks with eigenvalue $\lambda \neq 0$. It follows from eq (18) that $1+\lambda\Delta t$ lies in or on the circle with center $1+\alpha_{\max}\Delta t=1-|\alpha_{\max}|\Delta t$ and radius $|\alpha_{\max}|\Delta t$. Inequality (15) for Δt then implies that $1+\lambda\Delta t$ lies in or on the unit circle. Suppose, for a particular value $\widetilde{\Delta t}$ of Δt and for nonzero λ, that

$$|1+\lambda\widetilde{\Delta t}|=1.$$

Then, for $\Delta t<\widetilde{\Delta t}$,

$$|1+\lambda\Delta t|<1. \tag{27}$$

Hence, if inequality (15) is replaced by

$$\Delta t<\frac{1}{|\alpha_{\max}|}, \tag{28}$$

inequality (27) is guaranteed for any nonzero eigenvalue. The corresponding parts of $\mathbf{m}'$ accordingly converge to zero (Varga 1962), and the integration process based on eq (8) is stable.

3. STABILITY IN THE PRESENCE OF STEADY SOURCES AND A PENETRABLE BOUNDARY

Assume that all sources are steady and lie inside the region, that there are no sinks inside the region, and that the flow of tracer across the boundary is outward only. The full eq (6) must be used; that is,

$$\frac{d\mathbf{m}(t)}{dt}=\mathbf{A}\mathbf{m}(t)+\mathbf{S},$$

where the source vector, $\mathbf{S}$, is independent of time.

In the case $\mathbf{S}=\mathbf{O}$, the total mass cannot increase; therefore,

$$\sum_i \frac{dm_i}{dt}=\sum_{i,j}\alpha_{ij}m_j\leq 0 \tag{29}$$

for any set of nonnegative masses m_j. If the special set, $m_j=m\delta_{jk}$, is substituted into eq (29), inequality (12) results; that is,

$$\sum_i \alpha_{ik}\leq 0, \qquad k=1,\ \ldots,\ N.$$

Inequalities (9) and (12) together imply that

$$|\alpha_{kk}|\geq\sum_{i\neq k}|\alpha_{ik}|, \qquad k=1,\ \ldots,\ N. \tag{30}$$

Further, if box k is on a penetrable part of the boundary, the total mass must decrease, so

$$|\alpha_{kk}|>\sum_{i\neq k}|\alpha_{ik}|. \tag{31}$$

This must be true for at least one value of k.

The matrix $\mathbf{A}$ may be taken to be irreducible (if it were not irreducible, the time evolution of a subset of the masses would be independent of the remaining masses). Inequalities (30) and (31) then imply that the matrix $\mathbf{A}$ is "irreducibly diagonally dominant"; its eigenvalues therefore satisfy the inequality (Varga 1962),

$$\mathrm{Re}\lambda<0. \tag{32}$$

The formal solution of eq (6) is

$$\mathbf{m}(t)=[\exp\ (\mathbf{A}t)-\mathbf{I}]\mathbf{A}^{-1}\mathbf{S}+\exp\ (\mathbf{A}t)\mathbf{m}(0),$$

which, in view of inequality (32), converges as $t\rightarrow\infty$ to

$$\mathbf{m}=-\mathbf{A}^{-1}\mathbf{S}.$$

Similar arguments show that inequality (32) must also be satisfied in the case of eq (8). After n time steps Δt,

$$\begin{aligned}\mathbf{m}(n\Delta t)&=(\mathbf{I}+\Delta t\mathbf{A})^n\mathbf{m}(0)+(\mathbf{I}+\Delta t\mathbf{A})^{n-1}\Delta t\mathbf{S}\\&\quad+(\mathbf{I}+\Delta t\mathbf{A})^{n-2}\Delta t\mathbf{S}+\ \ldots\ +\Delta t\mathbf{S}\\&=\frac{\mathbf{I}-(\mathbf{I}+\Delta t\mathbf{A})^n}{\mathbf{I}-(\mathbf{I}+\Delta t\mathbf{A})}\Delta t\mathbf{S}+(\mathbf{I}+\Delta t\mathbf{A})^n\mathbf{m}(0).\end{aligned}$$

Inequality (27) implies that $(\mathbf{I}+\Delta t\ \mathbf{A})^n$ tends to zero as $n\rightarrow\infty$, and the whole expression tends to the limit $-\mathbf{A}^{-1}\mathbf{S}$ (which is independent of Δt). Thus, the finite-difference equation [eq (8)] is stable.

4. EXAMPLE—TWO-DIMENSIONAL MODEL OF THE STRATOSPHERE

In this section, we demonstrate how the preceding methods can be applied to the two-dimensional eddy diffusion model of the stratosphere proposed by Gudiksen et al. (1968). These authors used a numerical scheme based on the differential form of the continuity equation [eq (5)].

In the following derivation of a numerical form of the mass transfer equation, several approximations and physical assumptions are made. These are justified in the course of an analogous derivation done by Reed and German (1965), whose terminology we adopt where appropriate.

Equation (4) for the mass current, $\bar{\mathbf{j}}$, may be rewritten in the form

$$\bar{\mathbf{j}}=\bar{c}\bar{\mathbf{v}}-\rho\mathbf{K}\nabla\left(\frac{\bar{c}}{\rho}\right) \tag{33}$$

where $\bar{c}=\rho\,\bar{\chi}$ is the average concentration density of the tracer. Spreading in the longitudinal direction is rapid compared with spreading in the other directions and is assumed to result in a concentration of tracer nearly independent of longitude. The meridional and vertical components of the mass current are accordingly assumed to depend only on the meridional and vertical components of the gradient of the mean mass ratio $\bar{\chi}$. In a spherical coordinate system,

$$\nabla\left(\frac{\bar{c}}{\rho}\right)=\frac{1}{r}\frac{\partial}{\partial\phi}\left(\frac{\bar{c}}{\rho}\right)\hat{\phi}+\frac{\partial}{\partial z}\left(\frac{\bar{c}}{\rho}\right)\hat{z}.$$

Here $r=a+z$, where a is the radius of the earth, z is the height above the earth's surface, and ϕ is the latitude. Since $z\ll a$, it is a good approximation to replace r by a, as will be done in later equations.

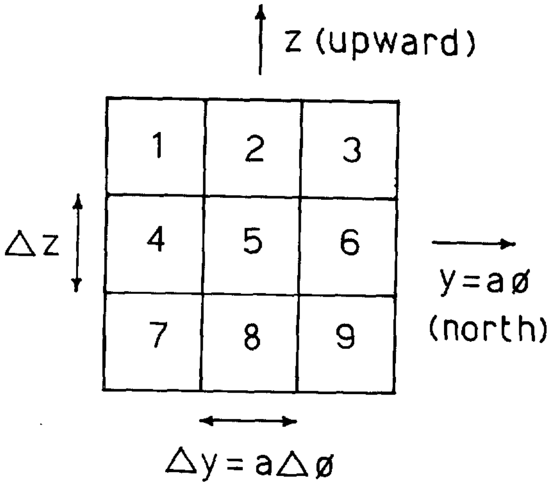

FIGURE 1.—A grid representing a set of neighboring boxes. The longitudinal direction extends perpendicular to the page.

If we further assume that ρ is a function of z only, we find that the meridional and vertical components of $\bar{\mathbf{j}}$ are

$$\bar{j}_y=\bar{c}(\bar{v}-\Gamma K_{yz})-K_{yy}\frac{\partial\bar{c}}{\partial y}-K_{yz}\frac{\partial\bar{c}}{\partial z}$$

and (34)

$$\bar{j}_z=\bar{c}(\bar{w}-\Gamma K_{zz})-K_{zz}\frac{\partial\bar{c}}{\partial z}-K_{zy}\frac{\partial\bar{c}}{\partial y},$$

where

$$y=a\phi,$$

$$\Gamma=-\frac{1}{\rho}\frac{d\rho}{dz},$$

and $\bar{v}$ and $\bar{w}$ and K_{yy}, $K_{yz}=K_{zy}$ and K_{zz} are the components of $\bar{\mathbf{v}}$ and $\mathbf{K}$, respectively. The last two terms of each component in eq (34) represent direct diffusion and cross diffusion, respectively. The first terms are due to winds; note that the transformation from spherical polar to two-dimensional Cartesian coordinates has introduced extra terms with the same mathematical form as winds.

Equation (34) is an appropriate starting point from which to develop numerical solutions having the properties of mass conservation, nonnegative masses, and stability. There are many possible numerical systems ensuring these properties. The following particular system is a simple, straightforward one.

The stratosphere is divided into boxes for which the boundaries are orthogonal surfaces of constant z and constant y at intervals of Δz and Δy, respectively. The rate of change of mass in a box due to winds and eddy diffusion must be calculated. The mass current at the face of a box may depend upon the position in the face because of spatially varying $\bar{\mathbf{v}}$ or $\mathbf{K}$. To obtain the mass flux through a face, we use for simplicity the zero-order term of a Taylor expansion for $\bar{\mathbf{j}}$. Thus, the mass flux across a face is the appropriate component of the mass current along the middle of the face, times the face area. The horizontal mass flux from the box centered at (y, z) to the box at $(y+\Delta y, z)$ is

$$\bar{j}_y(y+\tfrac{1}{2}\Delta y,z)\Delta z 2\pi a\cos\left(\frac{y+\frac{1}{2}\Delta y}{a}\right).$$

Similarly, the vertical mass flux from the box at (y, z) to the box at $(y, z+\Delta z)$ is

$$\bar{j}_z(y,z+\tfrac{1}{2}\Delta z)2\pi a\Delta y\cos\left(\frac{y}{a}\right).$$

The terms in parentheses after $\bar{j}_y$ and $\bar{j}_z$ indicate where the currents are to be evaluated. We must express $\bar{j}_y(y+\tfrac{1}{2}\Delta y,z)$ and $\bar{j}_z(y,z+\tfrac{1}{2}\Delta z)$ in a finite-difference form that ensures that conditions (9), (10), and (11) or (12) are satisfied. Consider the system of boxes as shown in figure 1. Let m_i represent the mass enclosed by box i, and let c_i be the concentration at the center. First we give an expression for the change in m_5 in a time Δt; then the rationale for the form of this expression is detailed. The change in m_5 is found from

$$m_5(t+\Delta t)=m_5(t)$$

$$-\left\{\begin{bmatrix}c_5(\bar{v}-\Gamma K_{yz}) & \text{if } \bar{v}-\Gamma K_{yz}>0\\ c_6(\bar{v}-\Gamma K_{yz}) & \text{if } \bar{v}-\Gamma K_{yz}<0\end{bmatrix}\right.$$

$$-K_{yy}\frac{c_6-c_5}{\Delta y}$$

$$\left.-\begin{bmatrix}K_{yz}\dfrac{\frac{1}{2}(c_3-c_6)+\frac{1}{2}(c_5-c_8)}{\Delta z} & \text{if } K_{yz}>0\\ K_{yz}\dfrac{\frac{1}{2}(c_2-c_5)+\frac{1}{2}(c_6-c_9)}{\Delta z} & \text{if } K_{yz}<0\end{bmatrix}\right\}_{(y+\frac{1}{2}\Delta y,\,z)}$$

$$\times\Delta z 2\pi a\cos\left(\frac{y+\frac{1}{2}\Delta y}{a}\right)\Delta t$$

$$+\left(\begin{array}{l}\text{analogous terms due to fluxes through}\\ \text{the faces bordering 2, 4, and 8}\end{array}\right)$$

$$+S_5\Delta t. \tag{35}$$

The notation $(y+\tfrac{1}{2}\Delta y,z)$ outside of the braces means that the wind and eddy diffusion coefficients are evaluated at this point. The form of the terms due to fluxes through the faces bordering 2, 4, and 8 is analogous to that shown for face 6. Explicit expressions may be obtained using the above set of boxes rotated through 90°, 180°, or 270°. S_5 describes sources for box 5.

This equation simply expresses (in approximate form) the fact that the rate of change of mass in a box is equal to the net flux across the boundaries plus a source term. It employs the first forward-difference formula [eq (7)] to approximate the time derivative $\partial m/\partial t$ and employs the simple but valid finite-difference approximations for the spatial derivatives $\partial\bar{c}/\partial y$ and $\partial\bar{c}/\partial z$. Note also that the effective wind is made to multiply the concentration of the box from which it is blowing.

The sign-dependent choices in eq (35) and the particular choices of finite-difference expressions are designed to ensure that conditions (9), (10), and (11) or (12) hold. To show that these conditions hold, we first substitute masses for concentrations. For simplicity, we set the concentration at the center of the box equal to the average concentration throughout the box; that is $c_i=m_i/V_i$, where V_i is the volume of box i. [The box centered at (y, z) has volume $2\pi a\Delta z\Delta y\cos(y/a)$.] Thus, eq (35) becomes an expression for the change in tracer mass in a box as a function of the masses in neighboring boxes.

After some rearrangement for computational convenience, eq (35) becomes

$$
\begin{aligned}
m_5(t+\Delta t)&=m_5(t)\\
&-\left\{\begin{bmatrix}\dfrac{m_5}{V_5}\bar{v}' & \text{if } \bar{v}'>0\\[2mm] \dfrac{m_6}{V_6}\bar{v}' & \text{if } \bar{v}'<0\end{bmatrix}-K'_{yy}\left(\frac{m_6}{V_6}-\frac{m_5}{V_5}\right)\right.\\
&\left.-\begin{bmatrix}K'_{yz}\left(\dfrac{m_3}{V_3}-\dfrac{m_8}{V_8}\right) & \text{if } K'_{yz}>0\\[2mm] K'_{yz}\left(\dfrac{m_2}{V_2}-\dfrac{m_9}{V_9}\right) & \text{if } K'_{yz}<0\end{bmatrix}\right\}_{(y+\frac{1}{2}\Delta y,\, z)}\\
&+(\text{analogous terms due to fluxes through the faces bordering 2, 4, and 8})\\
&+S_5\Delta t, \qquad (36)
\end{aligned}
$$

where

$$\bar{v}'=(\bar{v}-\Gamma K_{yz})A\Delta t,$$

$$K'_{yy}=\left(\frac{K_{yy}}{\Delta y}-\frac{|K_{yz}|}{2\Delta z}\right)A\Delta t,$$

$$K'_{yz}=\frac{K_{yz}}{2\Delta z}A\Delta t,$$

and

$$A=\Delta z 2\pi a\cos\left(\frac{y+\frac{1}{2}\Delta y}{a}\right).$$

The elements of the matrix **A** can be obtained by comparing eq (8) and (36). It is then possible to check that the above scheme has the properties of conservation of mass, nonnegative masses, and stability. Take the case in which there are no sources ($S_i=0$) and the boundaries are impenetrable. Because mass is simply transferred from one box to another, tracer mass is clearly conserved and eq (11) holds. For example, terms in braces in eq (36) are also contributions to $m_6(t+\Delta t)$, being *added* to $m_6(t)$. Because the wind and direct diffusion terms dominate the cross-diffusion terms, K'_{yy} at $(y+\frac{1}{2}\Delta y, z)$ and analogous quantities at the other borders are greater than zero. Thus, the coefficient of m_5 is negative, and eq (9) holds. However, the time step Δt must be sufficiently small that condition (28) is satisfied and m_5 remains nonnegative.

Equation (10) also holds. Masses in boxes 1, 3, 7, and 9 have nonnegative coefficients because of the form of the numerical expression for cross diffusion. The masses in boxes 2, 4, 6, and 8 receive direct diffusion from box 5, which dominates small, negative cross-diffusion terms; in eq (36), direct vertical diffusion dominates the explicit negative coefficients of m_8 or m_2. Thus, the coefficients of all masses other than m_5 are nonnegative, and condition (10) is satisfied. These arguments are not significantly altered if box 5 is on an impenetrable boundary.

If there are sources, mass is simply added to the box in question [see eq (8)]; this does not affect the matrix coefficients. However, if the boundary allows outward flow of tracer, then the above considerations are changed

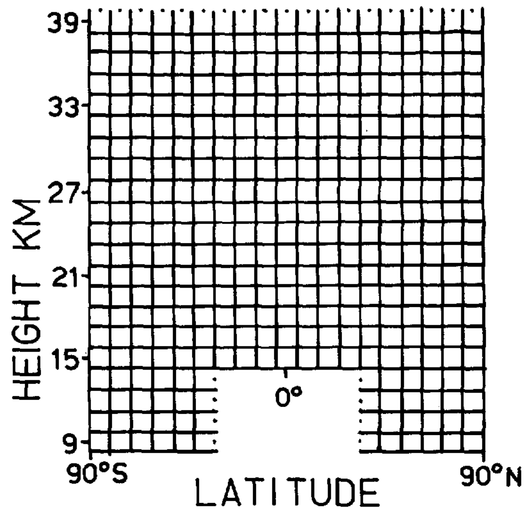

FIGURE 2.—A grid representing the division of the stratosphere into boxes. The boxes are generated by moving the grid around the earth along the lines of latitude. The bottom border crudely approximates the tropopause, through which matter can pass only outward via the "gap". The high upper boundary reduces the amount of mass flowing out of the top of the model to about 0.005 of that passing through the gap for our particular source.

to the extent that the diagonal coefficient for any box on the boundary is more negative than if the boundary were impenetrable. This corresponds to allowing a fixed fraction of the tracer in the relevant box to cross the boundary in any time step. Thus, condition (12) rather than condition (11) is satisfied.

5. SAMPLE USE OF NUMERICAL METHODS

The methods detailed in section 4 have been applied to a form of the two-dimensional model of the stratosphere used by Gudiksen et al. (1968).

Equation (36) was used to follow the change with time in the distribution of tracer mass in the stratosphere with a time-independent point source. Boxes were assigned in the two dimensions of latitude and altitude, as shown in figure 2. Solid lines indicate impenetrable boundaries, while dotted lines indicate boundaries through which matter can escape. To obtain a steady result with the constant source in the limit $t\rightarrow\infty$, we assumed the eddy diffusion coefficients and winds to be time independent. Incorporation of their time dependence into the time evolution of the system is straightforward if desired. In our case, the values of the parameters given by Reed and German (1965) for January were adopted.

The eddy diffusion coefficients and winds were interpolated linearly in space to give the appropriate parameters at the center of the face between each pair of boxes. Values of parameters at heights above 27 km were assumed equal to those at 27 km.

A source of 1 g/s in the box centered at 24 km and 28.4°N was assumed. A time step of 0.1 days was chosen, satisfying condition (28). The results of a computer run using the above methods are illustrated in figures 3 and 4, which show contours based upon the concentrations in the various boxes.

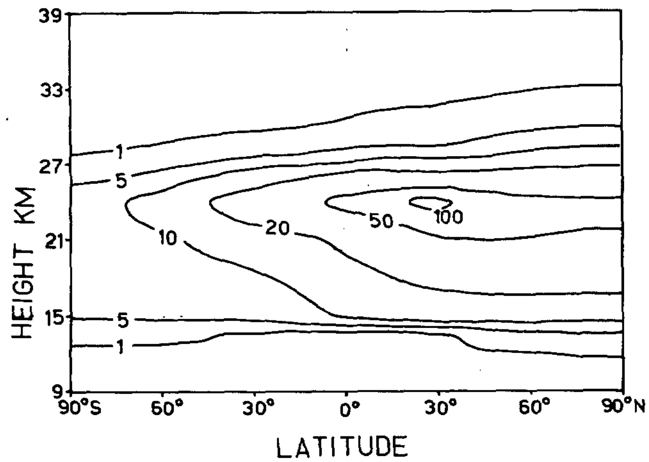

FIGURE 3.—A contour of the concentration of tracer in the stratosphere 200 days after the introduction of a source in the box at 24-km altitude and 28.4°N. Contour levels are in 10^{-24} mass units per cubic centimeter if the source introduces one mass unit per day.

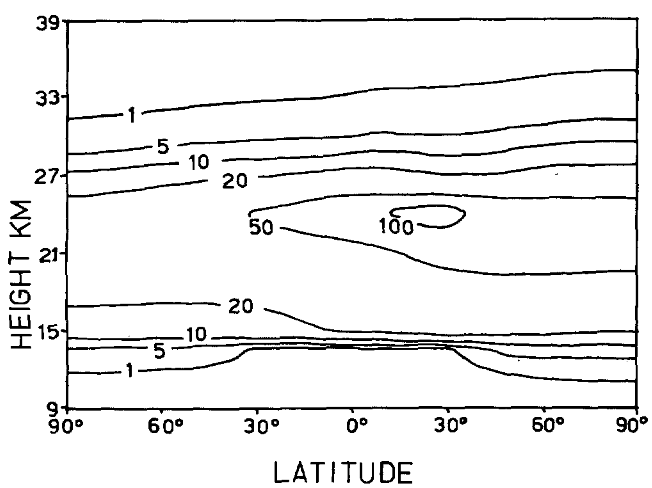

FIGURE 4.—Same as figure 3 for 400 days after introduction of source.

Several checks were made to see that the numerical methods were satisfying their claimed properties. The computer program was checked for negative masses at each time step and none was found. Moreover, the increase of total tracer mass in any time interval was equal, within the expected roundoff error of the computer, to the increase due to sources less the amount flowing out of the penetrable boundaries.

Finally, to check the convergence of the distribution, we solved the matrix equation for the steady-state solution directly. Setting $d\mathbf{m}/dt=0$ in eq (6) gives the equilibrium mass distribution

$$\hat{\mathbf{m}}=-\mathbf{A}^{-1}\mathbf{S}. \qquad (37)$$

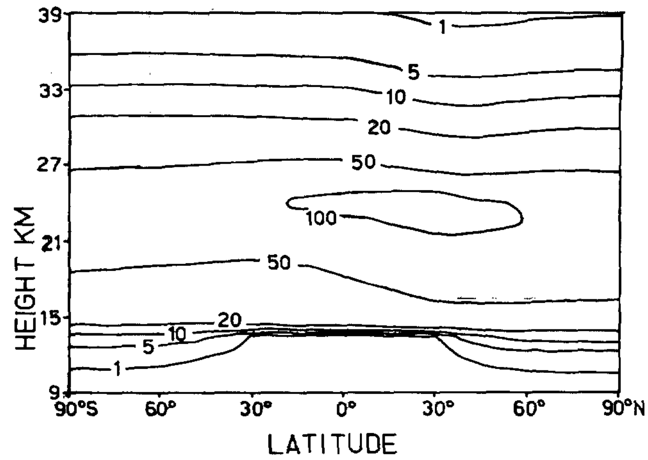

FIGURE 5.—Equilibrium concentrations of tracer in the stratosphere calculated using eq (37) with a source in the box at 24-km altitude and 28.4°N. Units are as in figure 3.

The existence of a unique equilibrium set of masses naturally depends on $\mathbf{A}$ having no time dependence—hence the use of time-independent eddy diffusion coefficients and winds in tracing the time evolution of $\mathbf{m}$. Using a Gaussian elimination method to find $\mathbf{A}^{-1}$, we determined the final distribution $\hat{\mathbf{m}}$. The results are contoured in figure 5. After 3–4 yr of time evolution, $\mathbf{m}$ becomes virtually indistinguishable from $\hat{\mathbf{m}}$, demonstrating satisfactory convergence.

ACKNOWLEDGMENTS

We wish to thank H. Messel and the Science Foundation for Physics at Sydney University for supporting this work and Hugh Comins for helpful remarks.

REFERENCES

Arakawa, Akio, "Computational Design for Long-Term Numerical Integration of the Equations of Fluid Motion. Two-Dimensional Incompressible Flow. Part I," *Journal of Computational Physics*, Vol. 1, No. 1, Academic Press, Inc., New York, N.Y., Jan. **1966**, pp. 119–143.

Bellman, Richard, *Introduction to Matrix Analysis*, McGraw-Hill Book Company, Inc. New York, N.Y., **1960**, 328 pp. (See pp. 191–194.)

Gudiksen, Paul H., Fairhall, A. W., and Reed, Richard J., "Roles of Mean Meridional Circulation and Eddy Diffusion in the Transport of Trace Substances in the Lower Stratosphere," *Journal of Geophysical Research*, Vol. 73, No. 14, July **1968**, pp. 4461–4473.

Hinze, J. O., *Turbulence: An Introduction to its Mechanism and Theory*, McGraw-Hill Book Company, Inc., New York, N. Y., **1959**, 506 pp. (See p. 25.)

Reed, Richard J. and German, Kenneth E., "A Contribution to the Problem of Stratospheric Diffusion by Large-Scale Mixing," *Monthly Weather Review*, Vol. 93, No. 5, May **1965**, pp. 313–321.

Varga, Richard S., *Matrix Iterative Analysis*, Prentice-Hall, Inc., Englewood Cliffs, N.J., **1962**, 322 pp. (See pp. 16, 265, 23.)

[*Received January 16, 1973; revised May 15, 1973*]